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2D dislocation dynamics in thin metal layers

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Abstract

The paper deals with a discrete dislocation dynamics study of plastic deformation in a thin film caused by thermal mismatch with its substrate. A unit cell analysis is carried out, with dislocations in the film being represented by line singularities in an isotropic linear elastic medium. Their mutual interactions as well as the interactions with the interface and the free surface are accounted for by means of a coupled dislocation dynamics-finite element technique. The formulation includes a set of constitutive rules to model generation, glide, annihilation and pinning of dislocations at point obstacles. The simulation tracks the evolution of the dislocation structure as thermal stress builds up as well as during relaxation under constant temperature, leading to dense dislocation distributions near the interface and a dislocation-free zone along the stress-free surface of the film.

Keywords: 2D dislocation dynamics; Plastic deformation; Thin metal layers

1. Introduction

The development and subsequent relaxation of stresses in thin layers has attracted much attention in recent years. Part of the interest is related to experimental observations of striking size effects for film thicknesses on the order of a micrometer or less, with thin films seeming to have considerably larger yield strengths than thicker ones. Certainly, the size effect cannot be captured by standard continuum plasticity since this does not include a material length scale.

When the film thickness is so small that is on the same order of magnitude as the charateristic dimensions of dislocation structure or spacings, the discreteness of dislocations needs to be taken in account. Indeed, several models of dislocations in thin films (e.g. [1,2]) have been put forward that explain how plastic relaxation can depend sensitively on the film thickness.

This paper aims at presenting a simulation technique that allows these models to be refined. We apply a method that was recently developed by Van der Giessen and Needleman [3] to solve boundary value problems in discrete dislocation plasticity. It uses a superposition of two contributions: the infinite medium solution for individual dislocations in infinite space and a non-singular solution that enforces the boundary conditions, and which is obtained from a linear elastic finite element solution. This approach enables the investigation of the dynamics of dislocations in the film with due account of the free surface and the interface with the substrate. Attention is confined here to single crystal films, and the elastic mismatch between film and substrate. After a brief summary of the actual unit cell model and the method of analysis, we present some results for different film thicknesses.

2. Model and method of solution

We consider a thin film on an infinitely thick substrate which will be cooled down and possibly kept at this temperature for a certain time. Thermal stress will build up during the thermal history due to the difference in thermal expansion between the film and the substrate. To be specific we will use the thermal expansion coefficient of Si for the substrate ($\alpha_s = 4.2 \times 10^{-6}\,\mathrm{K}^{-1}$) and the one for Al in the film ($\alpha_f = 23.2 \times 10^{-6}\,\mathrm{K}^{-1}$). Differences between elastic properties are neglected at this time, so that both the materials are governed by the thermo-elastic relation

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + (C - \tfrac{2}{3}\mu)\varepsilon_{kk}\delta_{ij} - 3C\alpha\Delta T\delta_{ij} \quad (1)$$

with the bulk modulus $C = 70\,\mathrm{GPa}$, the shear modulus $\mu = 26\,\mathrm{GPa}$ and with $\alpha = \alpha_f$ for the film and $\alpha = \alpha_s$ for the substrate. It is assumed that the thermal expansion in one of the two directions in the plane of the film is constrained, so that it suffices to describe the deformation of the system in two dimensions, with plane strain in the third direction. We take the film to be infinitely long and periodic, so that we can

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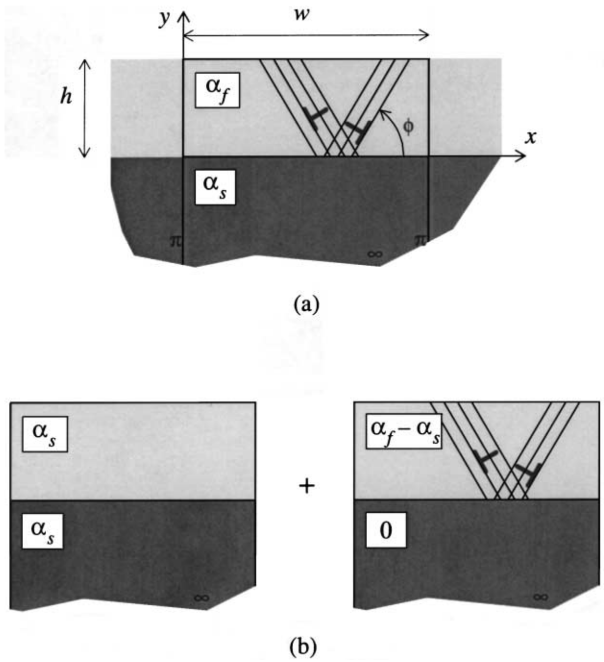

Fig. 1. (a) Unit cell in the two-dimensional film–substrate system. (b) First decomposition of the problem. The solution of the second part uses another decomposition, following [3].

identify a unit cell of width w as shown in Fig. 1a. The displacements u_i therefore have to satisfy the periodicity conditions

$$u_1(x+w,y)-u_1(x,y)=\alpha\Delta T w,$$
$$u_2(x+w)-u_2(x)=0 \tag{2}$$

with the (x, y)-coordinates according to Fig. 1a.

Within the framework of this two-dimensional study, plastic deformation in the film is taken to occur by the motion of edge dislocations on two slip systems, with slip planes inclined at $\pm 60^\circ$ from the film surface. The substrate is taken to remain elastic and the interface is treated as an impenetrable barrier for the dislocations. Dislocations are treated as line defects in an otherwise isotropic elastic medium [4,5].

The deformation history is carried out in an incremental manner. At each time step, an increment in temperature is applied, the dislocation arrangement is updated and finally the stress and strain state is updated. Postponing the discussion of the evolution of the dislocation structure, we first present the method to calculate the stress, strain and displacement fields in a given dislocated state for the current temperature change ΔT from the initial temperature.

For simplicity in implementing the boundary conditions, the problem is first decomposed in two linearly additive parts, as illustrated in Fig. 1b. The first part, identified as $()^{\mathrm{th}}$, describes the unconstrained thermal expansion of substrate and film as if they have the same coefficient of thermal expansion, $\alpha_{\mathrm{f}}=\alpha_{\mathrm{s}}$ and are without dislocations. The solution is $\varepsilon_{ij}^{\mathrm{th}}=\alpha_{\mathrm{f}}\Delta T\delta_{ij}$ and $\sigma_{ij}^{\mathrm{th}}=0$, both for the film and the substrate. The second part $()'$ corrects for the actual thermal expansion difference, by considering the constrained thermal expansion of a film with thermal expansion coefficient $\alpha=\alpha_{\mathrm{f}}-\alpha_{\mathrm{s}}$ on a substrate with $\alpha=0$. This part of the problem also accounts for the presence of the dislocations. The total solution is the sum of the two

$$u_i=u_i^{\mathrm{th}}+u_i',\qquad \sigma_{ij}=\sigma_{ij}^{\mathrm{th}}+\sigma_{ij}',\qquad \varepsilon_{ij}=\varepsilon_{ij}^{\mathrm{th}}+\varepsilon_{ij}.$$

The $()'$ fields for the second part are solved for by using the method for boundary value problems proposed in [3]. According to this method, the problem is again decomposed in two linearly additive parts so that the displacement, stress and strain field in the film are written as

$$u_i'=\tilde{u}_i+\hat{u}_i,\quad \sigma_{ij}'=\tilde{\sigma}_{ij}+\hat{\sigma}_{ij},\quad \varepsilon_{ij}'=\tilde{\varepsilon}_{ij}+\hat{\varepsilon}_{ij},$$

where the $(\tilde{\ })$ fields are the superposition of the fields of the individual dislocations as if they were in an infinite medium (e.g. [4,5])

$$\tilde{u}_i=\sum_I u_i^{(I)},\qquad \tilde{\sigma}_{ij}=\sum_I \sigma_{ij}^{(I)},$$
$$\tilde{\varepsilon}_{ij}=\sum_I \varepsilon_{ij}^{(I)}\quad (I=1,\ldots,n),$$

where n is the number of dislocations in the cell. These fields also account for the contributions of all the replicas of the dislocation in the other cells making up the film. This sum over all replicas is carried out analytically, as shown in (unpublished research), in order to avoid artificial dislocation patterning (see [3]). Special attention has been paid to the displacement fields when dislocations leave the free surface, in order that the correct step is left at the surface during the simulation.

The $(\hat{\ })$ fields represent the image fields that correct for the boundary conditions. Essentially, these are the free surface conditions

$$\sigma_{12}(x,h)=\sigma_{22}(x,h)=0,$$

where h is the film thickness, and conditions at the bottom of the substrate to prevent rigid body motions. Periodic boundary conditions are prescribed to the lateral sides. The $(\tilde{\ })$ fields are periodic by construction, so that pure periodicity conditions can be applied for the $(\hat{\ })$ fields. Since the $(\hat{\ })$ fields are smooth, the corresponding boundary value problem can be solved conveniently by, for instance, the finite element method.

The incremental change of the dislocation arrangement is governed by a set of constitutive rules for their motion, annihilation and generation. The driving force for all these mechanisms is the Peach–Koehler force acting on each dislocation. For dislocation the glide component of this force is calculated from

$$f^{(I)}=n_k\left(\hat{\sigma}_{kl}+\sum_{J\neq I}\sigma_{kl}^{(J)}\right)b_l$$

where n_i is the normal to the slip plane on which the dislocation lives and b_i is the Burgers vector (the magnitude is taken to be $b = 0.25$ nm). Dislocations glide on their slip planes according to the drag relation $f^{(I)} = Bv^{(I)}$ in which $v^{(I)}$ the dislocation velocity and B the drag coefficient (which we take here to have the value $B = 10^{-4}$ Pa s, typical for in aluminum. As it is not clear exactly how dislocations nucleate in thin films, we assume here that nucleation can occur at random positions inside the film. The criterion we use for dislocation nucleation is that when the Peach–Koehler force exceeds a critical value $\tau_{\mathrm{nuc}} b$ during a time span of t_{nuc}, a dislocation dipole is generated. The sources are distributed randomly over each slip plane and have random strengths; the mean value is $\tau_{\mathrm{nuc}} = 25$ MPa, while $t_{\mathrm{nuc}} = 10$ ns. The distance between the generated dislocations is taken so that their mutual attractive force is $\tau_{\mathrm{nuc}} b$. Annihilation takes place when two opposite-signed dislocations approach each other within a critical distance $L_{\mathrm{e}} = 6b$ and is simulated by removal of the two dislocations from the system.

3. Results

As a demonstration, the results of two simulations are presented, which differ only in the film thickness: $h = 1$ μm or $h = 0.5$ μm. The width of the unit cell is $w = 2$ μm in both cases. Potentially active slip planes at both orientations are equally spaced inside the cell at a distance of $50b$, giving a total of 276 slip planes. Sources are placed at a random position, one on each slip plane.

The temperature is decreased linearly in time from 600 to 300 K. The time for this we take to be 6 μs to minimize computing times. Each time step in the simulation is $\Delta t = 0.25$ ns.

At the starting temperature, the film is taken to be free of mobile dislocations. As the temperature decreases, an elastic tensile stress builds up in the film and after a temperature change of $\Delta T = -20$ K, the stress is large enough for the first source to nucleate a pair of dislocations. One of the dislocations glides towards the interface, where it will get blocked, and the other glides towards the free surface, that will tend to attract the dislocation. With continued cooling, more sources are activated. In addition, sources get activated by neighbouring dislocations because of their stress singularity, and this leads to an avalance of dislocations that relax the stress in the film.

Fig. 2 shows the distribution of the in-plane stress component σ_{xx} in the film with $h = 1$ μm and part of the substrate after cooling by $\Delta T = -300$ K, and the corresponding dislocation distributions. The stresses are normalized by the elastic stress, $\sigma_{\mathrm{e}} = 200$ MPa, that would be in the film without plastic relaxation. The dislocation distributions show three characteristic zones in the film: (i) one close to the interface, where many dislocations are piled-up; (ii) one near the free surface, where dislocations are almost completely absent; and (iii) an intermediate layer where dislocations are randomly distributed and apparently not structured. Closer examination of the dislocation structures in the first zone near the interface reveals that they add up to typical misfit super-dislocations with a net Burgers vector parallel to the interface. Because of this, the stress inside this zone tends to be rather high, and on average of the same order of magnitude as σ_{e}. The stresses in the top two zones have been almost completely relaxed by dislocation motion.

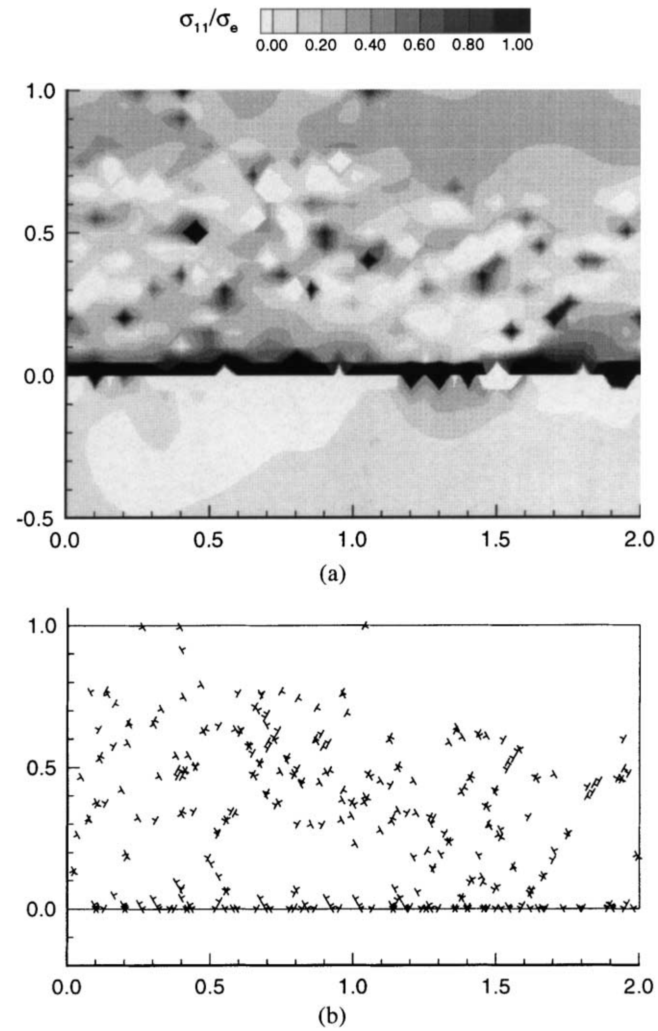

Fig. 2. (a) Stress in x-direction and (b) dislocation distribution in the 1 μm thick film after cooling by 300 K.

Similar results for the thinner film after the same amount of cooling are shown in Fig. 3. Comparison with Fig. 2 shows that the thickness of the dislocation-free zone is roughly the same as for the thicker film, ≅ 0.2 μm. Also the near-interface layer appears to have roughly the same thickness, ≅40 nm.

The fact that these special layers do not scale with the film thickness indicates that there is a size effect. This effect is illustrated in Fig. 4 in terms of the evolution of the average lattice strain (related to stress) in the film in the x-direction

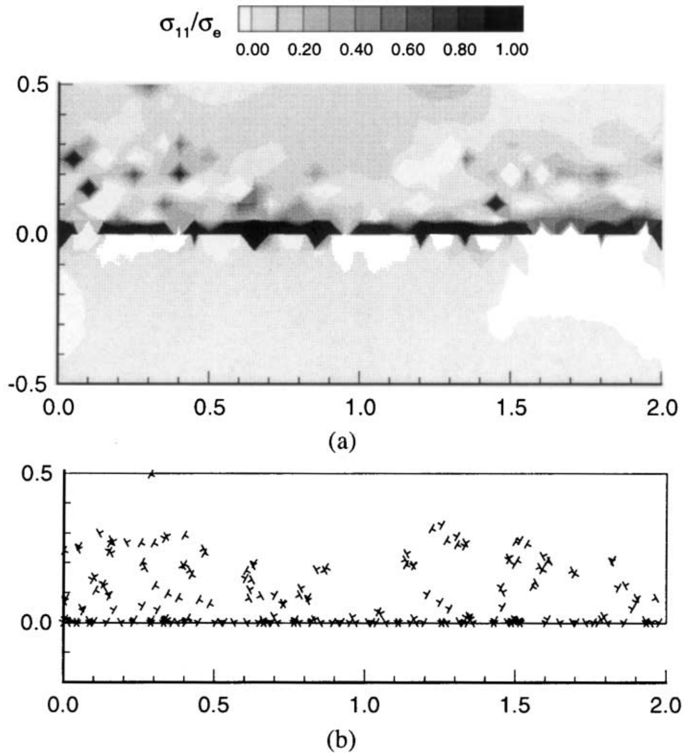

Fig. 3. (a) Stress in x-direction and (b) dislocation distribution in the $0.5\,\mu$m thick film after cooling by 300 K.

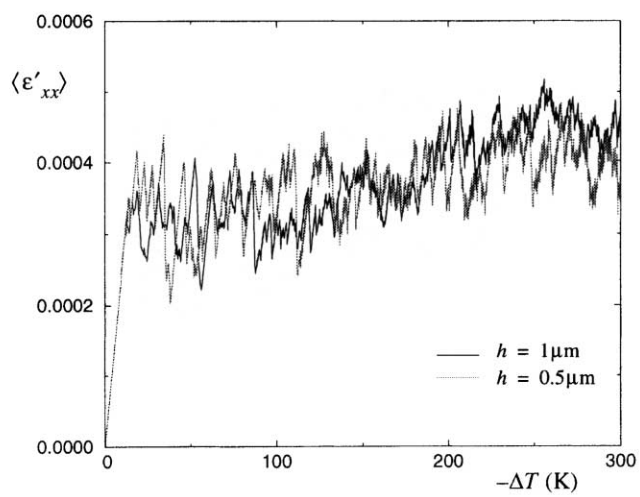

Fig. 4. Strain in x-direction averaged over the film thickness as a function of ΔT for films of different thicknesses.

(only the $()'$ part of the strain is shown). The yield point, i.e. the start of plastic deformation in the film, for a film thickness of $0.5\,\mu$m is higher than for $h = 1\,\mu$m. When the amount of plastic deformation increases, however, the hardening for the thinner film appears to be smaller. This is probably due to the fact that the source density is higher for the thinner film.

4. Conclusion

A two-dimensional methodology has been presented for dislocation dynamics simulation of plastic relaxation in thin films on elastic substrates. Preliminary results have been presented which demonstrate the thickness dependence for films with thicknesses around $1\,\mu$m. This is associated with the formation of two boundary layers in the film: a dislocation-free zone near the free surface and a "hard" boundary layer near the interface where dislocations pile up. The thicknesses of these layers is the same for the two film thicknesses considered here. Future work will explore the thickness dependence more carefully and compare this with experimental findings and theoretical considerations [1,2].

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